

Extreme points of the set of density matrices with positive partial transpose

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We present a necessary and sufficient condition for a finite dimensional density matrix to be an extreme point of the convex set of density matrices with positive partial transpose with respect to a subsystem. We also give an algorithm for finding such extreme points and illustrate this by some examples.

The density matrices describing states of a bipartite quantum system are uniquely classified as being either *separable* or *entangled*. However, it may be a non-trivial task in practice to classify a given density matrix. One simple method which can sometimes prove a density matrix to be entangled, and which is especially useful in systems with Hilbert spaces of low dimensions, is due to A. Peres [1]. Peres noted that a separable density matrix must remain positive when a partial transposition is performed with respect to one of the subsystems. In general the set of density matrices that have positive partial transpose, called PPT states for short, is larger than the set of separable matrices, but in low dimensions the difference between these two sets is small. In particular, for a system composed of one subsystem of dimension 2 and one subsystem of dimension 2 or 3, the two sets are known to be identical [2, 3].

A particular approach to the question of separability is to characterize geometrically the different sets of matrices as subsets of the real Hilbert space of hermitian matrices [4]. Thus, the set of all density matrices is a compact convex set \mathcal{D} , with the set of separable density matrices, \mathcal{S} , and the set of PPT matrices, \mathcal{P} , which we will call the *Peres set*, as convex subsets. The Peres criterion states that $\mathcal{S} \subset \mathcal{P} \subset \mathcal{D}$. We have presented elsewhere a numerical method for deciding whether a density matrix is included in \mathcal{S} by computing the distance to the closest separable density matrix [5, 6].

There are two complementary ways to characterize a convex set. One way is to specify its *extreme points*. Thus, every point in a compact convex set of finite dimension d has an expansion as a convex combination of $d + 1$ extreme points, while an extreme point cannot be written as a convex combination of other points in the set. The other way is to identify the set by conditions, typically algebraic equations and inequalities, that define whether or not a given point belongs to the set. For example, the convex set \mathcal{D} may be defined by its extreme points, which are the pure states (one dimensional projections), or equivalently by the conditions of hermiticity, positivity and unit trace. In general there is no simple relation between these two descriptions of a convex set.

It is interesting to note that the convex sets \mathcal{S} and \mathcal{P} have

simple characterizations in the complementary ways just described. Thus, the extreme points of \mathcal{S} are well known, they are the pure product states of the two subsystems, but there is no (known) effective test for membership of \mathcal{S} . In contrast, testing for membership of \mathcal{P} is easy, because $\mathcal{P} = \mathcal{D} \cap \mathcal{D}^P$, where the superscript P denotes partial transposition, but the extreme points of \mathcal{P} are not completely known.

The purpose of the present paper is to study the difference between the two sets \mathcal{S} and \mathcal{P} by studying the extreme points of \mathcal{P} . The extreme points of \mathcal{S} are also extreme points of \mathcal{P} , because they are extreme points of \mathcal{D} and $\mathcal{S} \subset \mathcal{P} \subset \mathcal{D}$. But in general \mathcal{P} is larger than \mathcal{S} and has additional extreme points, which are unknown and which make the whole difference between the two sets.

The extreme points of \mathcal{P} that are not pure product states are interesting also as examples of entangled PPT states. In fact, because $\mathcal{S} \subset \mathcal{P}$, a separable extreme point of \mathcal{P} must be an extreme point of \mathcal{S} and hence a pure product state. It is easy to verify that any pure state which is not a product state, is not in \mathcal{P} and is therefore entangled. Thus, every extreme point of \mathcal{P} which is not a pure product state, is entangled and has rank higher than one. A stronger lower bound on the ranks of entangled PPT states is actually known [7].

We will in the following specify a criterion for uniquely identifying the extreme points of \mathcal{P} and we will describe an algorithm for finding such points. The method is demonstrated by some examples.

To be more specific we consider a composite quantum system with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ of finite dimension $N = N_A N_B$, where A and B denote the two subsystems. Then \mathcal{D} is the set of density matrices on \mathcal{H} ,

$$\rho \in \mathcal{D} \Leftrightarrow \rho = \rho^\dagger, \quad \rho \geq 0, \quad \text{Tr} \rho = 1 \quad (1)$$

A subset is the Peres set \mathcal{P} ,

$$\rho \in \mathcal{P} \Leftrightarrow \rho \in \mathcal{D} \text{ and } \rho^P \in \mathcal{D} \quad (2)$$

where ρ^P is the partial transpose of ρ with respect to any one of the subsystems, say system B . A subset of \mathcal{P} is \mathcal{S} , the set

of separable density matrices,

$$\rho \in \mathcal{S} \Leftrightarrow \rho = \sum_k p_k \rho_k^A \otimes \rho_k^B, \quad p_k > 0, \quad \sum_k p_k = 1 \quad (3)$$

Thus, \mathcal{S} is the *convex hull* of the product states of the two subsystems, and its extreme points are the *pure* product states.

To develop the method we need for finding the extreme points of \mathcal{P} we will first apply it to \mathcal{D} , the full set of density matrices, with the pure states as extreme points. We recall some definitions and elementary facts.

Every $\rho \in \mathcal{D}$ is hermitian and has a spectral decomposition

$$\rho = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i| \quad (4)$$

with real eigenvalues λ_i and orthonormal eigenvectors $|\psi_i\rangle$. The positivity condition $\rho \geq 0$ means that all $\lambda_i \geq 0$, or equivalently that $\langle\psi|\rho|\psi\rangle \geq 0$ for all $|\psi\rangle$, with $\langle\psi|\rho|\psi\rangle = 0$ if and only if $\rho|\psi\rangle = 0$. The orthogonal projection

$$P = \sum_{i, \lambda_i > 0} |\psi_i\rangle\langle\psi_i| \quad (5)$$

projects onto the *image* (or *range*) of ρ , whereas $1 - P$ projects onto the *kernel* of ρ , denoted by $\ker \rho$.

If ρ is not an extreme point of \mathcal{D} it is a convex combination

$$\rho = x\rho' + (1 - x)\rho'', \quad 0 < x < 1 \quad (6)$$

with $\rho', \rho'' \in \mathcal{D}$ and $\rho' \neq \rho''$. The identity

$$\langle\psi|\rho|\psi\rangle = x \langle\psi|\rho'|\psi\rangle + (1 - x) \langle\psi|\rho''|\psi\rangle \quad (7)$$

shows that $\rho \geq 0$ when $\rho' \geq 0$ and $\rho'' \geq 0$, thus proving the convexity of \mathcal{D} . More interestingly, it shows that

$$\ker \rho = \ker \rho' \cap \ker \rho'' \quad (8)$$

With P defined as in (5) we have therefore $P\rho P = \rho$, $P\rho'P = \rho'$, and $P\rho''P = \rho''$.

When (6) holds, the matrix $\sigma = \rho' - \rho$ is hermitian and nonzero, and $\text{Tr } \sigma = 0$, hence σ has both positive and negative eigenvalues. Moreover, $P\sigma P = \sigma$. Define

$$\tau(x) = \rho + x\sigma \quad (9)$$

for x real. Since σ has both positive and negative eigenvalues, so has $\tau(x)$ for large enough $|x|$. If $\rho|\psi\rangle = 0$ then $P|\psi\rangle = 0$ and $\sigma|\psi\rangle = P\sigma P|\psi\rangle = 0$, hence $\tau(x)|\psi\rangle = 0$ for all x . Therefore only the strictly positive eigenvalues of ρ can change when $x\sigma$ is added to ρ , and since they change continuously with x , they remain positive for x in a finite interval about $x = 0$.

We conclude that there exists an $x_1 < 0$ and an $x_2 > 0$ such that $\tau(x) \geq 0$ for $x_1 \leq x \leq x_2$, and $\tau(x) \not\geq 0$ for $x < x_1$ or $x > x_2$. At $x = x_1$ or $x = x_2$, $\tau(x)$ has at least one zero eigenvalue more than ρ .

We are now prepared to search systematically for extreme points of \mathcal{D} . Starting with an arbitrary $\rho_1 \in \mathcal{D}$ we define the

projection P_1 in the same way as we defined P from ρ in (5). If we can find a hermitian matrix σ solving the equation

$$P_1\sigma P_1 = \sigma \quad (10)$$

we define

$$\sigma_1 = \sigma - (\text{Tr } \sigma) \rho_1 \quad (11)$$

in order to have $P_1\sigma_1P_1 = \sigma_1$ and $\text{Tr } \sigma_1 = 0$. Clearly $\sigma = \rho_1$ is a solution of (10). If this is the only solution, then only $\sigma_1 = 0$ is possible, and it follows from the above discussion that ρ_1 is an extreme point. The number of linearly independent solutions of (10) is n_1^2 , where $n_1 = \text{Tr } P_1$ is the rank of ρ_1 . Hence, ρ_1 is an extreme point if and only if $n_1 = 1$ so that it is a pure state.

If ρ_1 is not an extreme point, then we can find $\sigma_1 \neq 0$ and define

$$\tau_1(x) = \rho_1 + x\sigma_1 \quad (12)$$

We increase (or decrease) x from $x = 0$ until it first happens that $\tau_1(x)$ gets one or more additional zero eigenvalues as compared to ρ_1 . We will know if we go too far, because then $\tau_1(x)$ will get negative eigenvalues. We choose ρ_2 as the limiting $\tau_1(x)$ determined in this way. By construction, ρ_2 has lower rank than ρ_1 .

We repeat the whole procedure with ρ_2 in place of ρ_1 , and if ρ_2 is not extreme we will find a ρ_3 of lower rank. Continuing in the same way, we must end up at an extreme point ρ_K , with $K \leq N$, since we get a decreasing sequence of projections,

$$I \supseteq P_1 \supset P_2 \supset \dots \supset P_K \quad (13)$$

of decreasing ranks $N \geq n_1 > n_2 > \dots > n_K = 1$.

We may understand the above construction geometrically. In fact, each projection P_k defines a convex subset $P_k \mathcal{D} P_k$ of \mathcal{D} , with ρ_k as an interior point. This subset consists of all density matrices on the n_k dimensional Hilbert space $P_k \mathcal{H}$, and if $n_k < N$ it is a flat face of the boundary of \mathcal{D} .

It is straightforward to adapt the above method and use it to search for extreme points of \mathcal{P} . Thus, we consider an initial matrix $\rho_1 \in \mathcal{P}$, characterized by two integers (n_1, m_1) , the ranks of ρ_1 and of the partial transpose ρ_1^P , since $\rho_1 \in \mathcal{P}$ means that $\rho_1 \in \mathcal{D}$ and $\rho_1^P \in \mathcal{D}$. We denote by P_1 the projection on the image of ρ_1 , as before, and we introduce Q_1 as the projection on the image of ρ_1^P . We have to solve the two equations

$$P_1\sigma P_1 = \sigma, \quad Q_1\sigma^P Q_1 = \sigma^P \quad (14)$$

To understand these equations it may help to think of σ as a vector in the N^2 dimensional real Hilbert space \mathcal{M} of $N \times N$ hermitian matrices with the scalar product

$$\langle A, B \rangle = \langle B, A \rangle = \text{Tr}(AB) = \sum_{i,j} A_{ij}^* B_{ij} \quad (15)$$

If \mathbf{L} is a linear transformation on \mathcal{M} , its transpose \mathbf{L}^T is defined by the identity $\langle A, \mathbf{L}^T B \rangle = \langle \mathbf{L}A, B \rangle$, and \mathbf{L} is symmetric if $\mathbf{L}^T = \mathbf{L}$. Partial transposition of $A \in \mathcal{M}$ permutes the matrix elements of A and is a linear transformation $\mathbf{\Pi}A = A^P$. It is its own inverse, and is an orthogonal transformation (it preserves the scalar product), hence $\mathbf{\Pi} = \mathbf{\Pi}^{-1} = \mathbf{\Pi}^T$. It also preserves the trace, $\text{Tr}(\mathbf{\Pi}A) = \text{Tr} A$. The projections P_1 and Q_1 on \mathcal{H} define projections \mathbf{P}_1 and \mathbf{Q}_1 on \mathcal{M} by

$$\mathbf{P}_1 A = P_1 A P_1, \quad \mathbf{Q}_1 A = Q_1 A Q_1 \quad (16)$$

These are both orthogonal projections: $\mathbf{P}_1^2 = \mathbf{P}_1$, $\mathbf{P}_1^T = \mathbf{P}_1$, $\mathbf{Q}_1^2 = \mathbf{Q}_1$, and $\mathbf{Q}_1^T = \mathbf{Q}_1$.

In this language the equations (14) may be written as

$$\mathbf{P}_1 \sigma = \sigma, \quad \bar{\mathbf{Q}}_1 \sigma = \sigma \quad (17)$$

with $\bar{\mathbf{Q}}_1 = \mathbf{\Pi} \mathbf{Q}_1 \mathbf{\Pi}$. Note that $\bar{\mathbf{Q}}_1$ is also an orthogonal projection: $\bar{\mathbf{Q}}_1^2 = \bar{\mathbf{Q}}_1$ and $\bar{\mathbf{Q}}_1^T = \bar{\mathbf{Q}}_1$. These two equations are equivalent to the single equation

$$\mathbf{P}_1 \bar{\mathbf{Q}}_1 \mathbf{P}_1 \sigma = \sigma \quad (18)$$

or equivalently $\bar{\mathbf{Q}}_1 \mathbf{P}_1 \bar{\mathbf{Q}}_1 \sigma = \sigma$. They restrict the hermitian matrix σ to the intersection between the two subspaces of \mathcal{M} defined by the projections \mathbf{P}_1 and $\bar{\mathbf{Q}}_1$. We shall denote by \mathbf{B}_1 the projection on this subspace, which is spanned by the eigenvectors with eigenvalue 1 of $\mathbf{P}_1 \bar{\mathbf{Q}}_1 \mathbf{P}_1$. Because the latter is a symmetric linear transformation on \mathcal{M} it has a complete set of orthonormal real eigenvectors and eigenvalues. All its eigenvalues lie between 0 and 1. We may diagonalize it in order to find its eigenvectors with eigenvalue 1.

Having found σ as a solution of (18) we define σ_1 as in (11). If $\sigma = \rho_1$ and $\sigma_1 = 0$ is the only solution, then ρ_1 is an extreme point of \mathcal{P} . If we can find $\sigma_1 \neq 0$, then we define $\tau_1(x)$ as in (12), and increase (or decrease) x from $x = 0$ until we reach the first value of x where either $\tau_1(x)$ or $(\tau_1(x))^P$ has at least one new zero eigenvalue. This special $\tau_1(x)$ we take as ρ_2 . By construction, when n_2 is the rank of ρ_2 and m_2 the rank of ρ_2^P , we have $n_2 \leq n_1$, $m_2 \leq m_1$, and either $n_2 < n_1$ or $m_2 < m_1$.

Next, we check whether ρ_2 is an extreme point of \mathcal{P} , in the same way as with ρ_1 . If ρ_2 is not extreme, then we can find a third candidate ρ_3 , and so on. We will reach an extreme point ρ_K in a finite number of iterations, because the sum of ranks, $n_k + m_k$, decreases in each iteration.

The geometrical interpretation of this iteration scheme is that the density matrices $\rho \in \mathcal{P}$ which satisfy the condition $\mathbf{B}_k \rho = \rho$ define a convex subset of \mathcal{P} having ρ_k as an interior point. This subset is either the whole of \mathcal{P} , or a flat face of the boundary of \mathcal{P} , which is the intersection of a flat face of \mathcal{D} and a flat face of \mathcal{D}^P .

The construction discussed above defines an algorithm for finding extreme points of \mathcal{P} , and gives at the same time a necessary and sufficient condition for a density matrix in \mathcal{P} to be an extreme point. Let us restate this condition:

A density matrix $\rho \in \mathcal{P}$ is an extreme point of \mathcal{P} if and only if the projection P which projects on the image of ρ and

the projection Q which projects on the image of ρ^P , define a combined projection \mathbf{B} of rank 1 in the real Hilbert space \mathcal{M} of hermitian matrices.

The algorithm deserves some further comments. In iteration k the projections P_k , Q_k and \mathbf{B}_k are uniquely defined by the density matrix ρ_k , but the matrix σ_k is usually not unique. In the applications discussed below we have simply chosen σ_k randomly. Clearly, more systematic choices are possible if one wants to search for special types of extreme points.

Another comment concerns the ranks (n, m) of a density matrix ρ and its partial transpose ρ^P if it is an extreme point. We can derive an upper limit on these ranks. The rank of the projection \mathbf{P} is n^2 and the rank of $\bar{\mathbf{Q}}$ is m^2 , thus, the equations $\mathbf{P}\sigma = \sigma$ and $\bar{\mathbf{Q}}\sigma = \sigma$ for the N^2 dimensional vector σ represent $N^2 - n^2$ and $N^2 - m^2$ constraints, respectively. The total number of independent constraints is $n_c \leq 2N^2 - n^2 - m^2$, and the rank of \mathbf{B} is $N^2 - n_c \geq n^2 + m^2 - N^2$. For an extreme point the rank of \mathbf{B} is 1, implying the inequality

$$n^2 + m^2 \leq N^2 + 1 \quad (19)$$

We have used our algorithm in numerical studies. In one approach we use as initial density matrix the maximally mixed state $\rho_1 = 1/N$ and choose in iteration k a random direction in the subspace $\mathbf{B}_k \mathcal{M}$. We list in Table 1 all the ranks of extreme points found in this way in various dimensions $N = N_A N_B$. We do not distinguish between ranks (n, m) and (m, n) since there is full symmetry between ρ and ρ^P .

$N_A \times N_B = N$	(n, m)	$n + m$
$2 \times 4 = 8$	(5,6)	11
$3 \times 3 = 9$	(6,6) (5,7)	12
$2 \times 5 = 10$	(7,7) (6,8)	14
$2 \times 6 = 12$	(8,9)	17
$3 \times 4 = 12$	(8,9)	17
$3 \times 5 = 15$	(10,11)	21
$4 \times 4 = 16$	(11,11) (10,12)	22
$3 \times 6 = 18$	(12,13)	25
$4 \times 5 = 20$	(14,14) (13,15)	28
$5 \times 5 = 25$	(17,18)	35

TABLE I: Typical ranks (n, m) for extreme points

We find only solutions of *maximal rank*, in the sense that increasing either n or m will violate the inequality (19). Maximal rank means that the constraints given by the equations $\mathbf{P}\sigma = \sigma$ and $\bar{\mathbf{Q}}\sigma = \sigma$ are mostly independent. Furthermore, we find only the most symmetric ranks, in the sense that $m \approx n$. For example, in the 4×4 system we find ranks (11, 11) and (10, 12), but not (9, 13), (7, 14) or (5, 15), which are also maximal.

The 3×3 system we have examined further in the following way. For one specific sequence $\rho_1, \rho_2, \dots, \rho_K$ with ρ_K extreme, we repeat the final step, keeping ρ_{K-1} fixed but choosing different directions in the subspace $\mathbf{B}_{K-1} \mathcal{M}$. We find

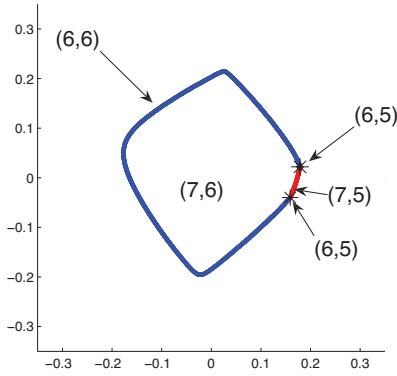


FIG. 1: Section through the boundary of \mathcal{P} , in 3×3 dimensions. A closed curve of extreme points surrounds a region of entangled PPT matrices of rank $(7, 6)$. The curve has two parts, characterized by ranks $(7, 5)$ and $(6, 6)$, joining at two rank $(6, 5)$ extreme points.

that every direction points directly towards an extreme point. Thus, ρ_{K-1} is an interior point of a flat face of the boundary of \mathcal{P} bounded by a hypersurface of extreme points. Fig. 1 shows a two dimensional section through this flat face.

This shows that extreme points of non-maximal rank do exist, and the fact that we do not find them in random searches just indicates that they define subsets of lower dimension than the extreme points of maximal rank (n, m) with $m \approx n$. Note that an extreme point which is not a pure product state cannot have arbitrarily low rank, since in [7] there is a proof that all PPT matrices of rank less than $N_0 = \min\{N_A, N_B\}$ are separable. This implies a lower limit of (N_0, N_0) for the ranks of an extreme point of \mathcal{P} which is not a pure product state. It is not known whether there exist entangled PPT states of the minimal rank N_0 .

Several of the low rank entangled PPT states that are known turn out, in our test, to be extreme points. Examples in 3×3 dimensions include the unextendible product basis state of rank $(4, 4)$ [8]; another state of rank $(4, 4)$ [9]; and explicit examples of rank $(5, 5)$ and $(6, 6)$ states [10].

The entangled PPT states first discovered [3], in 3×3 dimensions to be specific, are not extreme points of \mathcal{P} , but on the flat face defined by the corresponding projection **B** they seem to be completely surrounded by extreme points. Figure 2 is a two dimensional section chosen so as to show one such state (with parameter value $a = 0.42$, called here the “Horodecki state”), as a convex combination of two extreme points of \mathcal{P} . We would expect a two dimensional section through two extreme points of \mathcal{P} to show maximum difference between the sets \mathcal{S} and \mathcal{P} . Thus, this plot illustrates the fact that the difference is indeed very small in 3×3 dimensions.

In conclusion, the method discussed has the potential of producing a clearer picture of the difference between the two sets \mathcal{S} and \mathcal{P} and thereby the set of states with *bound entanglement*. We intend to follow up the work presented in this

paper by other numerical studies of composite systems of low Hilbert space dimensions.

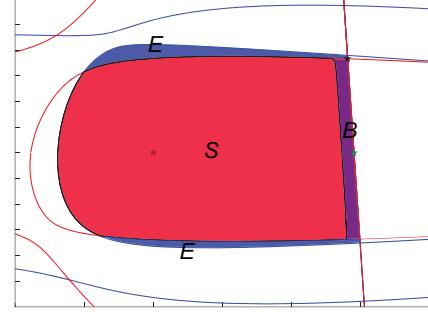


FIG. 2: Section through the set of density matrices in 3×3 dimensions. The star in the middle of a straight line is the “Horodecki state” (see text). It is a convex combination of two extreme points, one of which is plotted as a star. The maximally mixed state $1/N$ is the star close to the center. The separable matrices lie in the large (red) region marked S , the entangled PPT states in the (purple) region marked B , and the entangled non-PPT states in the two (blue) regions marked E . The lines are solutions of the equations $\det \rho = 0$ (blue) and $\det \rho^P = 0$ (red lines).

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